Eigenvalues from power–series expansions: an alternative approach

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Abstract. An appropriate rational approximation to the eigenfunction of the Schrödinger equation for anharmonic oscillators enables one to obtain the eigenvalue accurately as the limit of a sequence of roots of Hankel determinants. The convergence rate of this approach is greater than that for a well–established method based on a power–series expansions weighted by a Gaussian factor with an adjustable parameter (the so–called Hill–determinant method).

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1. Introduction

Power–series methods have proved to yield remarkably accurate eigenvalues of simple one–dimensional and central–field quantum–mechanical models [1–11]. There are basically two different approaches: on the one hand, the use of Dirichlet boundary conditions at the endpoints of a sufficiently wide interval [4, 10], on the other, the Hill–determinant method and its variants [1–9, 11]. In this paper we focus our attention on the latter that has been applied to a wide variety of problems, including the vibration–rotation spectra of diatomic molecules [5, 6, 8]. The success of this method commonly depends on the weight function which in many cases is an exponential function with a width parameter that affects the rate of convergence of the approach [1–3].

The purpose of this paper is to discuss an alternative approach that is less dependent on the width parameter or scaling factor. In sec. 2 we outline a well–known weighted power–series method. In sec. 3 we develop an alternative approach based on a rational approximation to that power series approach. In sec. 4 we apply both approaches to the pure quartic anharmonic oscillator. In sec. 5 we consider a rational potential with a singular point on the complex coordinate plane. Finally, in sec. 6 we draw conclusions.

2. Weighted power–series method

Consider the Schrödinger equation

$$\psi''(x) + [E - V(x)]\psi(x) = 0 \tag{1}$$

where the potential–energy function $V(x)$ can be expanded as

$$V(x) = \sum_{j=1}^{\infty} v_j x^{2j} \tag{2}$$

A well known approach for the calculation of eigenvalues and eigenfunctions is based on the ansatz

$$\psi(x) = e^{-ax^2} \sum_{j=0}^{\infty} c_j x^{2j+s} \tag{3}$$

where $s = 0$ or $s = 1$ for even or odd states, respectively. If this expansion satisfies the Schrödinger equation (1), then the coefficients c_j are polynomial functions of the energy E. It has been shown [1–3] that one can obtain the allowed energies (those consistent with square–integrable solutions) from the roots of

$$c_M(E) = 0, \ M = M_0, \ M_0 + 1, \ldots \tag{4}$$

The rate of convergence of the sequence of roots $E^{[M]}$ of this equation depends on the adjustable parameter a. If its value is far from optimal, the sequences may not converge at all.

3. The Hankel–Padé method

The Riccati Padé method is based on a rational approximation to the logarithmic derivative of the eigenfunction $f(x) = s/x - \psi'(x)/\psi(x)$ [12, 13]. An appropriate truncation condition determines the allowed energies to be the roots of Hankel determinants [12, 13]. The convergence rate of the sequences of such roots is remarkable and provides accurate eigenvalues with Hankel determinants of relatively small dimension.

Here we explore an alternative approach based on a rational approximation to $x^{-s}\psi(x)e^{ax^2}$:

$$\frac{\sum_{j=0}^{N+d} a_j x^{2j}}{\sum_{j=0}^{N} b_j x^{2j}} = \sum_{j=0}^{2N+d+1} c_j x^{2j} \tag{5}$$

Notice that we require that the Padé approximant with just $2N + d + 1$ adjustable parameters yields $2N + d + 2$ coefficients of the power series (3). As in the case of the Riccati–Padé method [12, 13] it leads to a quantization condition for the energy given by the roots of the Hankel determinants

$$H_D^d(E) = |c_{i+j+d-1}(E)|_{i,j=1}^{D} = 0 \tag{6}$$

where $D = N + 1 = 2, 3, \ldots$, and $d = 0, 1, \ldots$

4. Anharmonic oscillator

As an example consider the anharmonic oscillator

$$V(x) = x^4 \tag{7}$$

The first coefficients are:

$$
\begin{aligned}
c_1 &= a - \frac{E}{2} \\
c_2 &= \frac{a^2}{2} - \frac{Ea}{2} + \frac{E^2}{24}
\end{aligned}
\tag{8}
$$

and the first Hankel determinant is

$$H_2^0 = \frac{a}{30} - \frac{a^4}{12} - \frac{E}{60} + \frac{Ea^3}{6} - \frac{E^2 a^2}{8} + \frac{7E^3 a}{360} - \frac{E^4}{960} \tag{9}$$

Fig. 1 shows several sequences of roots of $H_D^0(E) = 0$ when $a = 0$. We appreciate that the phenomenon of multiple converging sequences of roots present in the RPM [12, 13] also appears in this case. It seems to be related to the Hankel determinant and to the rational approximation (either to the logarithmic derivative or to just a factor of the wave function). A straight line in Fig. 1 marks the sequence with the best convergence rate. One obtains similar sequences for other values of a. Notice that the standard method (4) [1–3] does not apply to the case $a = 0$.

Fig. 2 shows the logarithmic error $\log |E_{approx} - E_{exact}|$ of the sequences of roots of $H_D^0(E) = 0$ and $c_M(E) = 0$ for $a = 1$ in terms of the number of coefficients $M = 2D - 1$ required by the calculation. Straight lines show the overall trend of the logarithmic sequences. We appreciate that the Hankel sequence converges faster than the one for the standard approach. The "exact" result $E_{exact} = 1.0603620904841828996$ is simply a more accurate estimate of the eigenvalue provided by the RPM [12, 13].

Fig 3 shows the variation of the logarithmic error of the roots of $c_M(E) = 0$ with a for three values of M. We appreciate that the optimal value of the adjustable parameter for the quartic oscillator (7) is about $a \approx 2.5$.

It is not necessary to have the "exact" energy in order to estimate an optimal value of the adjustable parameter. If $E_n^{[k]}$ is the approximation of order k to the n–th

eigenvalue, we simply monitor the convergence of the sequence in terms of, for example, $\log |E_n^{[k+1]} - E_n^{[k]}|$, where $k = k_0, k_0 + 1, \ldots$.

5. Rational potential

Both the straightforward power–series method and the Hankel–Padé approach apply successfully to polynomial potentials as illustrated in the preceding section by means of a simple nontrivial example. In what follows we consider the rational potential

$$V(x) = x^2 + \lambda x^2/(1 + gx^2), \quad -\infty < \lambda < \infty, \, g > 0 \tag{10}$$

that has been studied by several authors [14–57]. Among the approaches applied to this model we mention perturbation theory [15, 22, 24, 30, 52], including the $1/N$ expansion [38, 42, 43], variational methods [14, 16, 34, 55, 57], and in particular the Rayleigh–Ritz method [14, 34, 55, 57]. One can easily obtain exact solutions to the Schrödinger equation with the potential (10) for some values of the parameters λ and g [17,19–23,25–28,35,37,39,41,43–49,51,57] that prove suitable for testing approximate methods.

The power series (2) converges only for $|x| < |x_g|$, where $x_g = \pm i/\sqrt{g}$ are the two poles of the potential–energy function on the imaginary axis of the complex x–plane. If $g \ll 1$ the eigenfunction is negligible for $|x| > |x_g|$ and the Hill–determinant method may yield reasonable results for the lowest energies and only after judicious truncation of the sequences of roots [5]. On the other hand, the expansion of the wavefunction in a power series of the variable $u = x^2/(1 + gx^2)$ leads to a successful approach for all values of g and λ [50].

Since the Hankel–Padé method is based on a rational approximation to the wavefunction, one expects that it takes into account the singularities properly, succeeding even for moderate values of g. In what follows we compare it with the weighted power–series method (3). First of all, notice that $V(x)/x^2 \to 1$ as $|x| \to \infty$ so that we expect $a = 1/2$ to be optimal [3] and choose this width–parameter value from

now on. We have verified that the Hankel–Padé approach yields reasonable results for other values of a such as, for example, $a = 0$, $a = 1$ and $a = 3/2$.

Table 1 shows the results of the Hankel–Padé calculation of the ground–state eigenvalue of the Schrödinger equation (1) with the rational potential (10) for $\lambda = 1$ and three values of g. Notice that present Hankel–Padé results are more accurate than those obtained earlier by means of the Rayleigh–Ritz variational method [14], and comparable to those provided by a kind of iterative solution of the Rayleigh–Ritz secular equation with an adjustable parameter [34]. There are much more accurate results in the literature; for example, Stubbins and Gornstein [55] obtained $E_0 = 1.3805318009380452343899500609$ and $E_0 = 1.2323507234060578138620699586 8$ for $g = 0.1$ and $g = 1$, respectively.

Table 2 shows results from the Hill–determinant method. A lack of entry means that we did not find any root in the interval $0.5 < E < 1.5$. Notice that while the Hankel–Padé approach converges smoothly the Hill–determinant method does not, even for $g = 0.1$. Besides, the latter approach does not give any reasonable result for $g = 1$. For $g = 0.1$ the roots of the Hill–determinant oscillate about the exact eigenvalue, giving the tightest bounds for $9 \leq M \leq 12$, before the sequence begins to diverge. Averaging the roots for $M = 10$ and $M = 11$ one estimates $E_0 = 1.38053181$ that is quite close to the exact eigenvalue. However, this strategy is only practical for sufficiently small values of g as discussed above. We have thus verified our earlier supposition that the Hankel–Padé method should correct a possible failure of the power–series approach caused by singular points of the potential–energy function in the complex coordinate plane.

6. Further comments and conclusions

Clearly, the results of the preceding sections show that

- The sequence of roots of the Hankel determinants (6) converges more smoothly than the sequence of roots of equation (4) for polynomial potentials.

- The rate of convergence of the sequence of roots of the Hankel determinants (6) is not so strongly dependent on the value of a as the sequence of roots of the standard approach (4). In fact, the former converges where the latter does not (even when $a = 0$).

- The Hankel–Padé method is preferable for the treatment of potential–energy functions with singularities in the complex coordinate plane that limit seriously the range of applicability of the power series.

- However, from a purely practical point of view it is worth noticing that when both approaches are successful, the calculation of the roots of the Hankel determinants typically requires more CPU time.

- There is more than one sequence of roots of the Hankel determinant (6) that converges towards a given eigenvalue. Present approach shares this curious phenomenon with the RPM [12, 13] and appears to be a feature of the Hankel determinants constructed from the coefficients of the power series coming from either the Riccati equation or the Schrödinger one.

The Schrödinger equation with the simple potential–energy functions discussed above can easily be treated by means of the Rayleigh–Ritz variational method and the basis set of eigenfunctions $\{\phi_n\}$ of the harmonic oscillator $\hat{H} = \hat{p}^2 + \omega^2 x^2$, where ω is an adjustable parameter. The problem reduces to the diagonalization of the Hamiltonian matrix $\mathbf{H}$ with elements $H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle$. The main advantage of this approach is that it provides upper bounds to all the eigenvalues [14, 34, 55, 57]. Besides, in some cases $H_{ij} = 0$ for all $|i - j| > k$, and the resulting secular equation with a band matrix can be treated as a recurrence relation. In this way one does not have to diagonalize a large matrix but simply to find the roots of a determinant of much smaller constant dimension [58]. This is precisely the case for the simple examples discussed above. However, this variational method may not be practical if the calculation of the matrix elements of the potential–energy function is too difficult. In that case the power–series methods and its variants may be preferable.

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Table 1. Hankel–Padé estimate of the ground–state eigenvalue of the Schrödinger equation with the rational potential (10) for $\lambda = 1$

D	$g = 0.1$	$g = 0.2$	$g = 1$
2	1.385	1.353120	1.21
3	1.380525	1.353123	1.23
4	1.3805318	1.3529481	1.232
5	1.3805322	1.3529489	1.2323
6	1.38053181	1.352948023	1.23234
7	1.3805318009377	1.352952	1.232348
8	1.38053180938043	1.352948022755	1.2323502
9	1.380531800938043	1.352948037359	1.2323506
10	1.38053180093804523	1.352948022753577	1.23235069
11	1.3805318009380452345	1.352948022753566	1.23235072
12	1.3805318009380452344	1.35294802275357088	1.232350721
13	1.3805318009380452344	1.35294802275357081	1.232350723
14		1.3529480227535708289	1.2323507233
15		1.3529480227535708284	1.23235072337
16		1.3529480227535708285	1.23235072339
17		1.3529480227535708284	1.232350723403
18		1.3529480227535708284	1.232350723405
19			1.2323507234057
20			1.23235072340595
21			1.23235072340602
22			1.232350723406047
23			1.232350723406054
24			1.232350723406056
25			1.232350723406057

Table 2. Hill–determinant estimate of the ground–state eigenvalue of the Schrödinger equation with the rational potential (10) for $\lambda = 1$

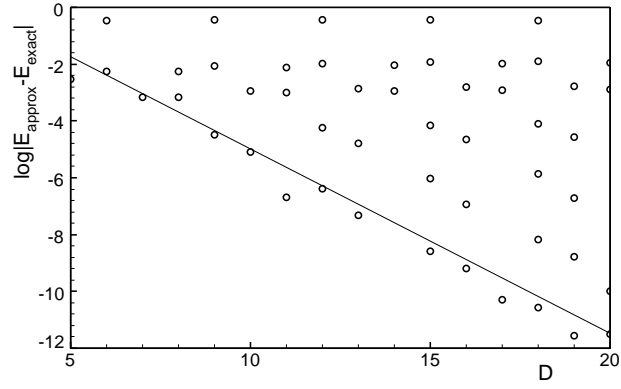| M	$g = 0.1$	$g = 0.2$
2	1.59	1.59
3	1.32	1.26
4	1.41	1.43
5	1.37	1.30
6	1.389	1.42
7	1.375	1.29
8	1.385	1.46
9	1.377	1.22
10	1.384	1.82
11	1.377	1.03
12	1.384	
13	1.376	
14	1.386	
15	1.373	
16	1.391	
17	1.364	
18	1.409	
19	1.337	
20	1.48	
21	1.25	

Figure 1. Sequences of roots of $H_D^d(E) = 0$ for the lowest eigenvalue of the quartic anharmonic oscillator (7) when $a = 0$
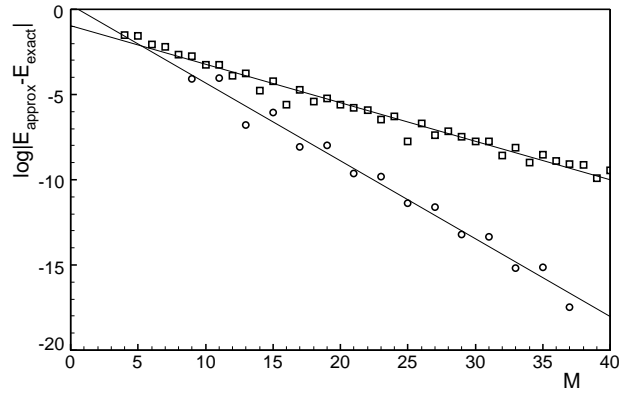

Figure 2. Sequences of roots of $H_D^d(E) = 0$ (circles) and $c_M(E) = 0$ (squares), $M = 2D - 1$, for the lowest eigenvalue of the quartic anharmonic oscillator (7) when $a = 1$
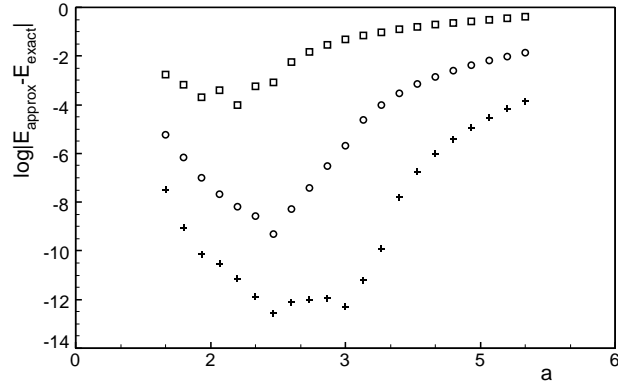
Figure 3. Logarithmic error of the roots of $c_M(E) = 0$ as function of a for $M = 9$ (squares), $M = 19$ (circles) and $M = 29$ (crosses) for the lowest eigenvalue of the quartic anharmonic oscillator (7)